A Journey from Cellular Automata and Kinetic Theory to Lattice Boltmann Models

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with P. Lallemand and I. Ginzburg,
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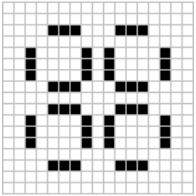
Cellular Automaton

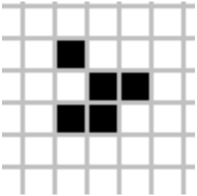
Cellular automa were introduced by John von Neumann in the 1940s and are defined on a regular grid by:

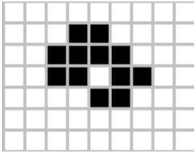
- the space dimension D,
- an internal state $S(t)$,
- a neigborhood N,
- a transition rule $T(S, S_N)$, such that $S(t+1) = T(S, S_N)(t)$.

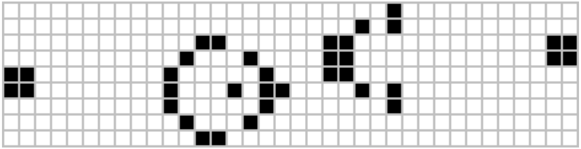
Usual neighborhoods: von Neuman (first neighbors on a square grid) and Moore (first and secon neighbors).

Game of life of John Conway in 1970.

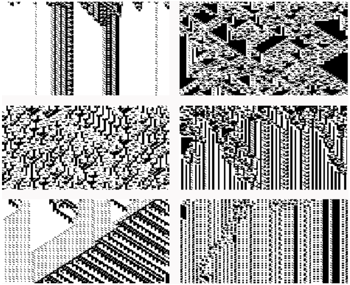


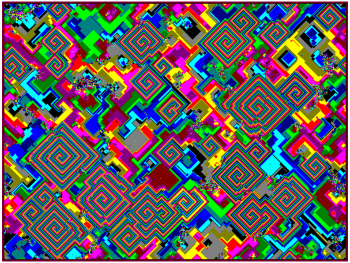






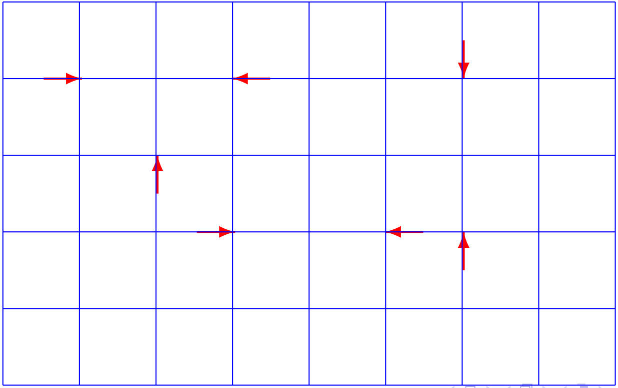
In the 1980s a lot of interest: S. Kaufmann, IMAG group, S. Wolfram,





and T. Toffoli and N. Margolus and their “wonderful machine”: "Cellular Automata Machines", by Tommaso Toffoli and Norman Margolus (MIT Press, 1987).

$[N, W, S, E]_{ij}^{t+1} = T([N_{i,j+1}, W_{i-1,j}, S_{i,j-1}, E_{i+1,j}]^t),$
with $T(S = S$ if $S \neq 0101$ nor 1010,
and $T(0101) = 1010$ and $T(1010) = 0101$.



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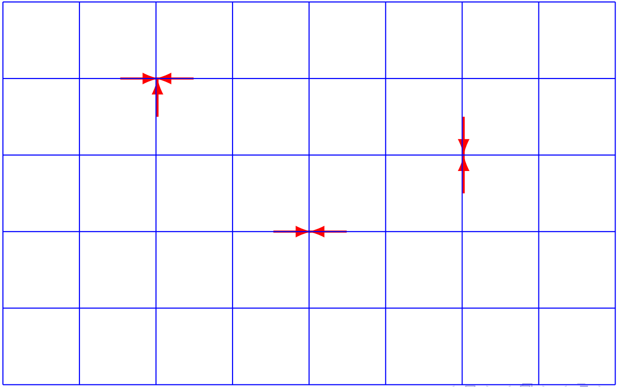

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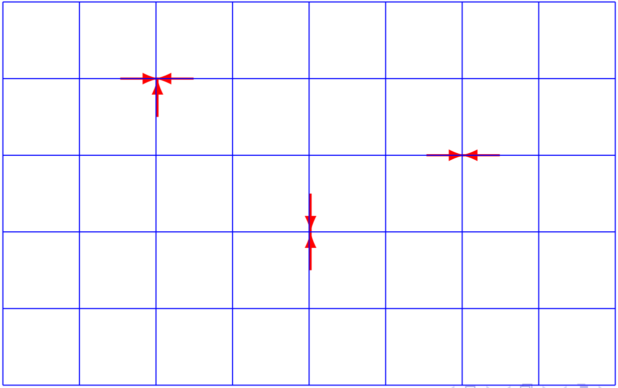

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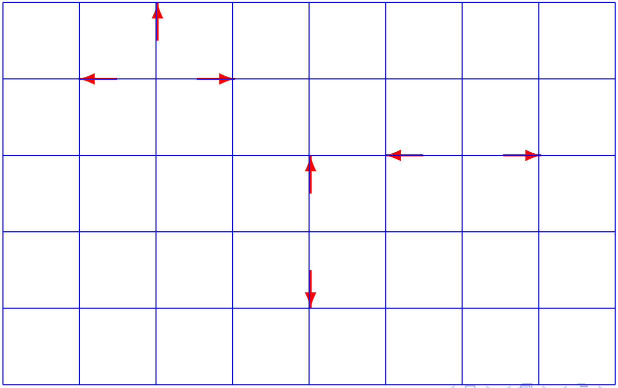


This CA is now known as HPP for J. Hardy, Y. Pomeau, and O. de Pazzis, “Time evolution of two-dimensional model system. I. Invariant states and time correlation functions”, *J. Math. Phys.* **14**, 1746-1759 (1973).

Denoting the four velocities $\vec{c}_1 = (1, 0)$, $\vec{c}_2 = (0, 1)$, $\vec{c}_3 = (-1, 0)$, and $\vec{c}_4 = (0, -1)$, the evolution equation can be written:

$$b_i(\vec{r} + \vec{c}_i, t + 1) - b_i(\vec{r}, t) =$$
$$(-1)^i [b_1 b_3 (1 - b_2)(1 - b_4) - b_2 b_4 (1 - b_1)(1 - b_3)](\vec{r}, t),$$

with the conservation of mass and momentum:

$$\rho = \sum_i b_i \text{ and } \vec{\jmath} = \rho \vec{u} = \sum_i b_i \vec{c}_i .$$

Denoting $f_i = \langle b_i \rangle$ and neglecting the correlations, one gets:

$$f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) =$$
$$(-1)^i [f_1 f_3 (1 - f_2)(1 - f_4) - f_2 f_4 (1 - f_1)(1 - f_3)](\vec{r}, t),$$

with

$$\rho = \sum_i f_i \text{ and } \vec{\jmath} = \rho \vec{u} = \sum_i f_i \vec{c}_i.$$

To be compared to the Boltzmann equation:

$$\partial_t f(\vec{r}, \vec{c}, t) + \vec{c} \cdot \nabla f(\vec{r}, \vec{c}, t) = \mathcal{C}(f).$$

Then the standard techniques developped for the Boltzmann equation and the discrete velocity models (Broadwell in the 1960s, Cabannes, Gatignol, from the mid 1970s) were adapted to the lattice gases.

1. It exists an equilibrium distribution $\{f_i^{eq}\}$ such that $\mathcal{C}(f_i^{eq}) = 0$ given by

$$f_i^{eq} = \frac{1}{1 + \exp(h + \vec{q} \cdot \vec{c}_i)},$$

$$\text{with} \sum_i f_i^{eq} = \rho \text{ and } \sum_i f_i^{eq} \vec{c}_i = \vec{\jmath}.$$

2. $\mathcal{C}$ is linearized in the neighborhood of $\{f_i^{eq}\}$.
3. $\{f_i^{eq}\}$ is Taylor expanded around $\vec{u} = 0$.
4. Then a Chapman-Enskog expansion of the evolution equation is performed.

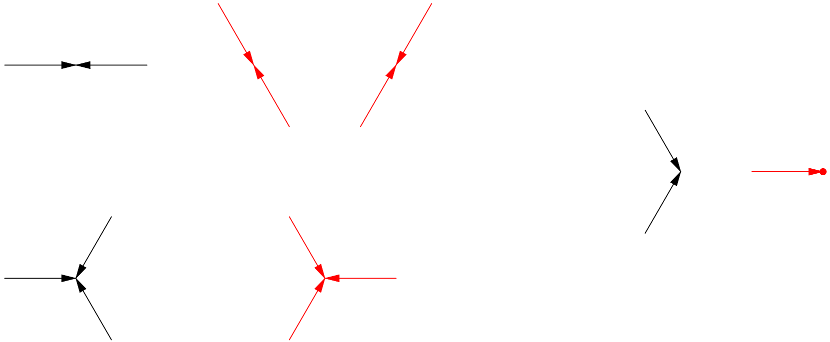
These steps give the following macroscopic equations:

$$\partial_t \rho + \nabla \cdot \vec{j} = 0,$$
$$\partial_t j_\alpha + \partial_\beta(\rho G(\rho) T_{\alpha\beta\gamma\delta} u_\gamma u_\delta) = \frac{c^2}{D}\partial_\alpha \rho + \partial_\beta(\psi(\rho) T_{\alpha\beta\gamma\delta}\partial_\gamma \rho u_\delta),$$

$$\text{with} \quad T_{\alpha\beta\gamma\delta} = \sum_i c_{i\alpha} c_{i\beta} (c_{i\gamma} c_{i\delta} - \frac{c^2}{D}\delta_{\gamma\delta}).$$

Isotropy is recovered iff $\sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} \sim \delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}$. For HPP the sum is proportional to $\delta_{\alpha\beta\gamma\delta}$ and its hydrodynamics is not isotropic.

U. Frisch, B. Hasslacher, and Y. Pomeau, “Lattice-gas automata for the Navier-Stokes equation”, *Phys. Rev. Lett.* **56**, 1505-1508 (1986).



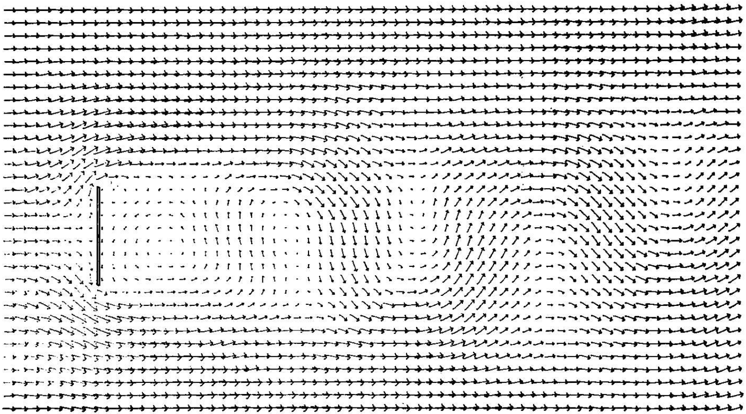
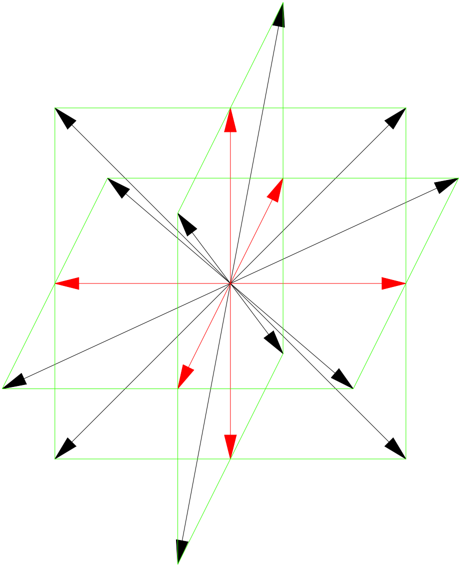


Fig. 2. — Écoulement obtenu dans les conditions de la figure 1 au temps $t = 5\,500$.

Fig. 2. — Flow under same conditions as in Figure 1, 500 *time steps later.*



D. d'Humières, P. Lallemand, and U. Frisch, "Lattice gas models for 3D hydrodynamics", *Europhys. Lett. 2*, 291-297 (1986).

Problems with lattice gases

1. complexity of building the collision table for FCHC:
   - HPP: 16 states,
   - FHP: 64 or 128 states,
   - FCHC: over 16 million states.
2. Lack of flexibility of the transport coefficients.
3. No Galilean invariance: recovered in the incompressible limit by rescaling time and viscosities by some term $g(\rho_0)$.
4. Spurious conserved quantites.
5. Noise.

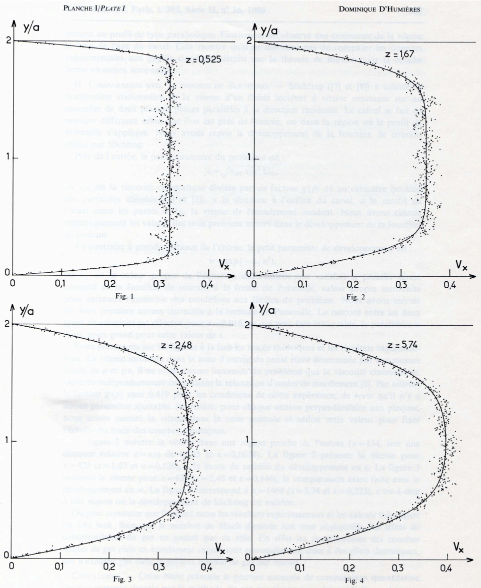


PLANCHE I/PLATE I
DOMINIQUE D'HUMIÈRES
y/a
2
1
0
z = 0,525
Vx
0
0,1
0,2
0,3
0,4
Fig. 1
z = 1,67
Fig. 2
z = 2,48
Fig. 3
z = 5,74
Fig. 4

First attempt: G. McNamara and G. Zanetti, “Use of the Boltzmann equation to simulate lattice- gas automata”, *Phys. Rev. Lett.* **61**, 2332–2335 (1988).

$$f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) =$$
$$(-1)^i [f_1 f_3 (1 - f_2)(1 - f_4) - f_2 f_4 (1 - f_1)(1 - f_3)](\vec{r}, t).$$

Second attempt in the line of the Broadwell model: J.E. Broadwell, “Shock structure in a simple discrete velocity gas”, *Phys. Fluids* **7**, 1243–1247 (1964).

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$$f_i(\vec{r}+\vec{c}_i, t+1) - f_i(\vec{r}, t) = (-1)^i [f_1 f_3 - f_2 f_4](\vec{r}, t).$$

Third attempt: F.J. Higuera, J. Jiménez, “Boltzmann approach to lattice gas simulations”, *Europhys. Lett.*, **9**, 663–668 (1989).

$$f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) = -[(\mathsf{A} \cdot (\mathbf{f} - \mathbf{f}^{eq}))_i](\vec{r}, t).$$

In the original paper A and $\mathbf{f}^{eq}$ were derived from the lattice gases models. Then the BGK model $\mathsf{A} = \mathsf{I}/\tau$ was developed followed by more sophisticated models.

- a cubic lattice in D dimensions,
- a set of Q velocities $(\vec{c}_q\delta x/\delta t)$ connecting nodes of the lattice and such that, for any $\vec{c}_q$ in the set, $\vec{c}_{\bar{q}} = -\vec{c}_q$ is also in the set,
- an associated set of particle densities $f_q(\vec{r}, t)$ $(\mathbf{f} = (f_q))$,
- an evolution equation for these particle densities:

$$f_q(\vec{r} + \vec{c}_q\delta x, t + \delta t) = f_q^*(\vec{r}, t) \equiv f_q(\vec{r}, t) + \mathcal{C}_q(\mathbf{f}(\vec{r}, t)),$$

where $\mathcal{C}$ is a collision term function of $\mathbf{f}$.

- D1Q3: $\{-1, 0, 1\}$,
- D2Q5: $\{(0, -1), (-1, 0), (0, 0), (1, 0), (0, 1)\}$,
- D2Q9: D2Q5 $\cup \{(-1, -1), (-1, 1), (1, -1), (1, 1)\}$,
- D3Q7: $\{(0, 0, 0), (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\}$,
- D3Q9: $\{(0, 0, 0), (\pm 1, \pm 1, \pm 1)\}$,
- D3Q13: $\{(0, 0, 0), (\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1)\}$,
- D3Q15: D3Q7 $\cup$ D3Q9,
- D3Q19: D3Q7 $\cup$ D3Q13,
- D3Q27: D3Q7 $\cup$ D3Q9 $\cup$ D3Q13,

Following Higuera et al. (1989), the collision term is done through a relaxation toward a given "attractor" $\mathbf{e}$ function of $\mathbf{f}$: $\mathcal{C}(\mathbf{f}) = -\mathcal{A} \cdot (\mathbf{f} - \mathbf{e}(\mathbf{f}))$, where $\mathcal{A}$ is a given collision operator.

- BGK (Bhatnagar-Gross-Krook) or SRT (Single-Relaxation-Time): $\mathcal{A} = \lambda \mathcal{I}$ $(\lambda = 1/\tau)$.
- MRT (Multiple-Relaxation-Time): $\mathcal{A}$ is defined by its eigenvalues (relaxation times) and its eigenvectors.
  - "Kinetic" models: eigenvectors based on the velocity set, $\mathbf{b}_{mnp} = (c_{qx}^m c_{qy}^n c_{qz}^p)$.
  - L-models (I. Ginzburg): based on the symmetric and antisymmetric components of $\mathbf{f}$.

Splitting the particle densities in their symmetric and antisymmetric components:

$$f_q^+ = \frac{(f_q + f_{\bar{q}})}{2}, \qquad f_q^- = \frac{(f_q - f_{\bar{q}})}{2},$$
$$f_q = f_q^+ + f_q^-, \qquad f_{\bar{q}} = f_q^+ - f_q^-.$$

the TRT evolution is given by

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [f_q - \lambda^+ (f_q^+ - e_q^+) - \lambda^- (f_q^- - e_q^-)](\vec{r}, t),$$

or with $\lambda^* = (\lambda^+ + \lambda^-)/2$ and $\delta\lambda = (\lambda^+ - \lambda^-)/2$

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [(1 - \lambda^*) f_q - \delta\lambda\, f_{\bar{q}} + \lambda^* e_q + \delta\lambda\, e_{\bar{q}}](\vec{r}, t),$$

The fundamental ingredient of the LB models is the existence of quantities conserved during the collision, for instance the mass:

$$\rho = \sum_q f_q = \sum_q f_q^*,$$

the momentum

$$\rho \vec{u} = \sum_q f_q \vec{c}_q = \sum_q f_q^* \vec{c}_q,$$

energy ...

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energy ...

The “attractor” of the relaxation (also called equilibrium) is restricted to be functions of the conserved quantities only. To satisfy the conservation laws, the equilibrium must be chosen such that:

$$\sum_q e_q = \rho,$$

for the mass,

$$\sum_q e_q \vec{c}_q = \rho \vec{u}.$$

for the momentum ...

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for the momentum ...

Dispersion Equation.

In a periodic domain, the solutions of the linearized evolution equations have the form:

$$\mathbf{f}(\vec{r}, t) = \Omega^{t/\delta t} \exp(i\vec{k} \cdot \vec{r}/\delta x)\mathbf{f}_0,$$

The population $\mathbf{f}$ after advection is given by

$$\mathbf{f}(\vec{r} + \vec{c}_q \delta x, t + \delta t) = \Omega e^{ik_q} \mathbf{f}(\vec{r}, t),$$

with $k_q = \vec{k} \cdot \vec{c}_q$. Using $\mathcal{K} = \mathrm{diag}(e^{ik_q})$ and $\mathbf{e} = \mathcal{E}\mathbf{f}$, it comes

$$(\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E})) \cdot \mathbf{f}_0 = \Omega \mathcal{K} \cdot \mathbf{f}_0.$$

Writing the system:

$$\Omega\,\mathbf{f}_0 = \mathcal{K}^{-1} \cdot (\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E})) \cdot \mathbf{f}_0,$$

the growth rates Ω are the eigenvalue of the matrix $\mathcal{K}^{-1} \cdot (\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E}))$.
When $k = 0$, $\Omega = 1$ for the conserved quantities. The expansion of Ω in power series of k around $k = 0$ gives the transport coefficients of the model and their errors as a function of k.
The LB model will be stable for a set of parameters defining $\mathcal{A}$ and $\mathcal{E}$ iff all the Ω are $|\Omega| \leq 1$ for all the values of $0 \leq \vec{k} \leq \pi$).
Taking $\Omega = 1$ and replacing k with ik, the roots of

$$\mathrm{Det}(\mathcal{K} - (\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E})))$$

for $\vec{k}$ perpendicular to a given boundary plane correspond to the Knudsen modes.

For the BGK models the evolution equation is given by

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [f_q - \lambda(f_q - e_q)](\vec{r}, t),$$

For $\lambda = 1$ this equation becomes

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = e_q(\vec{r}, t),$$

or

$$f_q(\vec{r}, t + \delta t) = e_q(\vec{r} - \vec{c}_q \delta x, t),$$

Projecting this equation on the conserved quantities, it comes

$$\rho(\vec{r}, t + \delta t) - \rho(\vec{r}, t) = \sum_q (e_q(\vec{r} - \vec{c}_q \delta x, t) - e_q(\vec{r}, t)),$$

The TRT evolution equation is given by

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [(1 - \lambda^*) f_q - \delta\lambda\, f_{\bar{q}} + \lambda^* e_q + \delta\lambda\, e_{\bar{q}}](\vec{r}, t),$$

For $\lambda^* = 1$ the TRT evolution equation becomes

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r}, t),$$

For $\lambda^* = 1$ the TRT evolution equation can also be written

$$f_q(\vec{r}, t + \delta t) = [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

For $\lambda^* = 1$ the TRT evolution equation can also be written

$$f_q(\vec{r}, t + \delta t) \quad = \quad [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

or

$$f_{\bar{q}}(\vec{r} - \vec{c}_q \delta x, t) \quad = \quad [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t),$$

For $\lambda^* = 1$ the TRT evolution equation can also be written

$$f_q(\vec{r}, t + \delta t) = [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

or

$$f_{\bar{q}}(\vec{r} - \vec{c}_q \delta x, t) = [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t),$$

then

$$\begin{aligned} f_q(\vec{r}, t + \delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t), \end{aligned}$$

Summing over q the equation

$$\begin{aligned} f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

gives

$$\begin{aligned} \rho(\vec{r}, t+\delta t) &= \sum_q [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda \sum_q [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

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gives also

$$\rho(\vec{r}, t+\delta t) = -\delta\lambda\, \rho(\vec{r}, t-\delta t) + \sum_q [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

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$$\begin{aligned} f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

gives also

$$\begin{aligned} \rho(\vec{r}, t+\delta t) &= -\delta\lambda\, \rho(\vec{r}, t-dt) \\ &+ \sum_q [(1+\delta\lambda\,)e_q^+ + (1-\delta\lambda\,)e_q^-](\vec{r} - \vec{c}_q \delta x, t), \end{aligned}$$

Summing over q the equation

$$\begin{aligned} f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q\delta x, t) \\ &- \delta\lambda\,[-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

gives finally a du Fort-Frankel scheme ($(1+\delta\lambda)/(1-\delta\lambda) = 2\Lambda^-$)

$$\frac{1}{2}(\rho(\vec{r}, t+\delta t) - \rho(\vec{r}, t-\delta t)) - \sum_q e_q^-(\vec{r} - \vec{c}_q\delta x, t) =$$

$$2\Lambda^- \sum_q (e_q^+(\vec{r} - \vec{c}_q\delta x, t) - \frac{1}{2}(e_q^+(\vec{r}, t+\delta t) + e_q^+(\vec{r}, t-\delta t))),$$

Summary

- The lattice Boltzmann method is based on standard tools of kinetic.
- LBM for hydrodynamics are compressible, but not "restricted to low Mach numbers".
- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- Open Questions.
  - Interfaces.
  - Clean inclusion of source terms.
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?

Summary

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